

Integrating Machine Learning and Multiscale Modeling in Biomedical Sciences

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We will present a new approach to develop a data-driven, learning-based framework for predicting outcomes of biophysical systems and for discovering hidden mechanisms and pathways from noisy data. We will introduce a deep learning approach based on neural networks (NNs) and on generative adversarial networks (GANs) for utilizing historical data to obtain functional priors and posteriors. Unlike other approaches that rely on big data, here we “learn” from small data by exploiting the information provided by the mathematical biophysics, e.g., conservation laws, reaction kinetics, etc., which are used to obtain informative priors or regularize the neural networks. We will demonstrate how we can train Biophysics-Informed Neural Networks (BINNs) from multifidelity/multimodality data, and we will present several examples of inverse problems, e.g., in systems biology for diabetes and in biomechanics for non-invasive inference of thrombus material properties. We will also discuss how operator regression in the form of DeepOnet can be used to accelerate inference based on historical data and only a few new data, as well its generalization and transfer learning capacity.